



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:53 AM UTC

PDB ID : 7MYA / pdb_00007mya
Title : Structure of proline utilization A with the FAD covalently-modified by 1,3-dithiolane
Authors : Tanner, J.J.; Campbell, A.C.
Deposited on : 2021-05-20
Resolution : 1.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

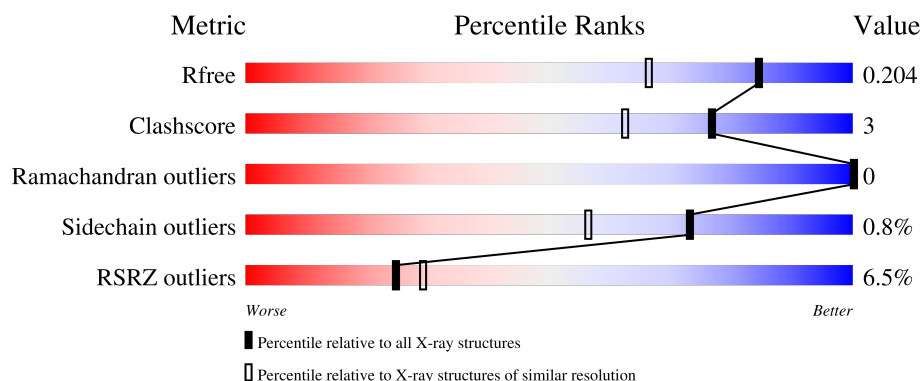
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1235	5% 92% 6%
1	B	1235	8% 91% 7%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20344 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

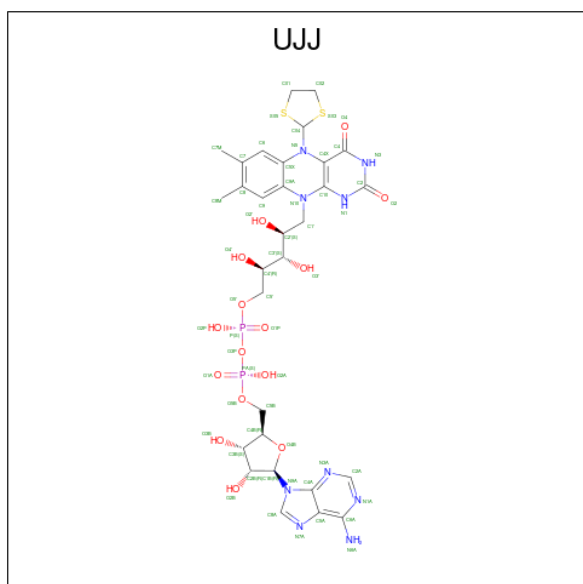
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1217	Total	C	N	O	S	0	17	0
			9063	5713	1615	1700	35			
1	B	1217	Total	C	N	O	S	0	15	0
			9042	5698	1616	1695	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4S)-5-[5-(1,3-dithiolan-2-yl)-7,8-dimethyl-2,4-dioxo-1,3,4,5-tetrahydrobenzo[g]pteridin-10(2H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (CCD ID: UJJ) (formula: C₃₀H₃₉N₉O₁₅P₂S₂) (labeled as "Ligand of Interest" by depositor).

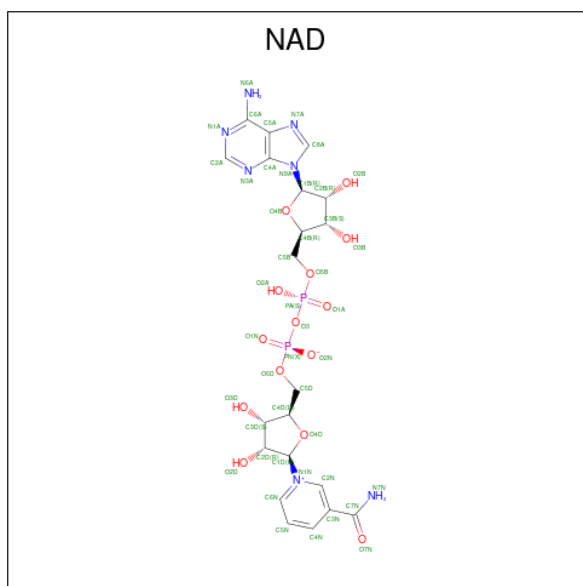


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			58	30	9	15	2	2	
2	B	1	Total	C	N	O	P	S	
			58	30	9	15	2	2	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P		
			44	21	7	14	2	0	0
4	B	1	Total	C	N	O	P		
			44	21	7	14	2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



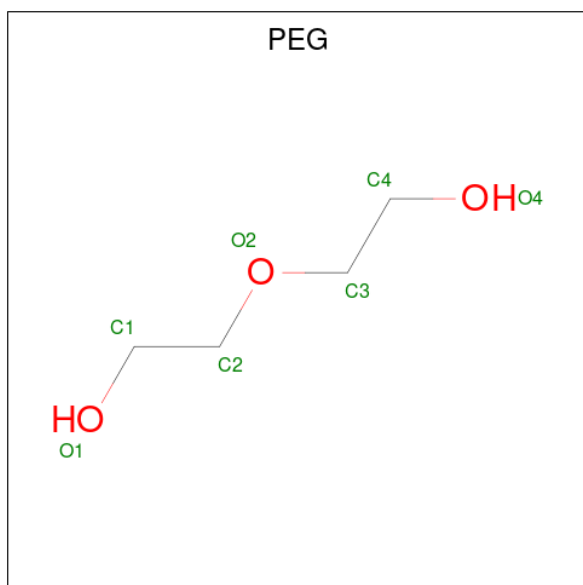
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



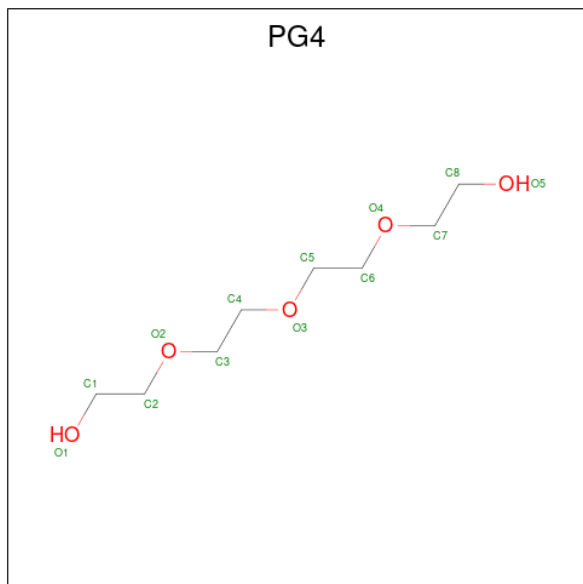
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

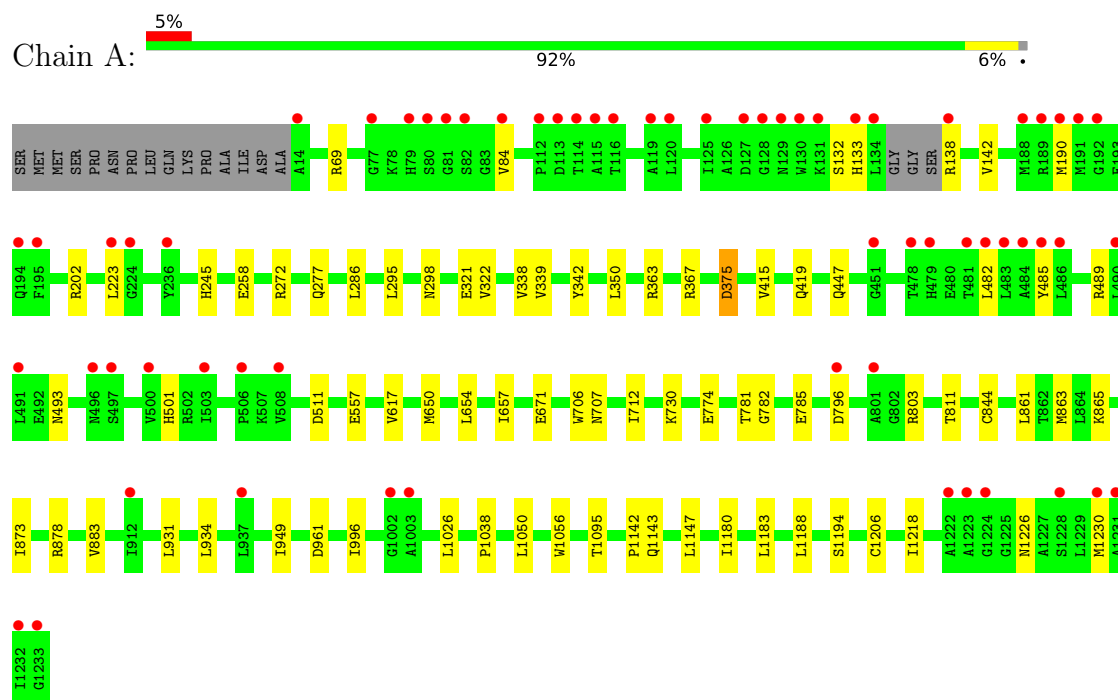
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	983	Total	O	0	0
			983	983		
9	B	941	Total	O	0	1
			941	941		

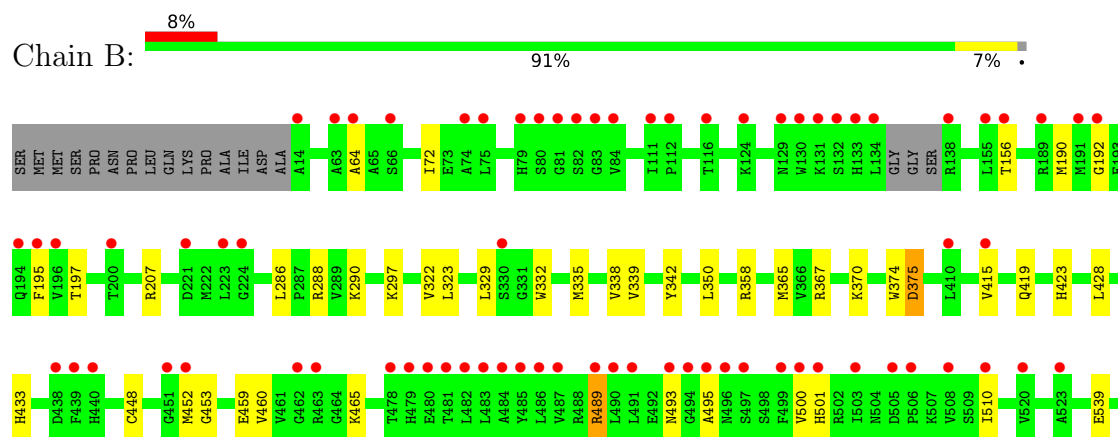
3 Residue-property plots [i](#)

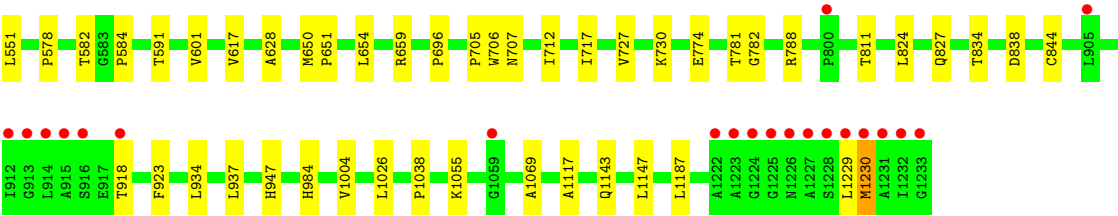
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.18Å 101.88Å 125.93Å 90.00° 106.49° 90.00°	Depositor
Resolution (Å)	46.94 – 1.56 46.94 – 1.56	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.94-1.56) 90.8 (46.94-1.56)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.176 , 0.205 0.175 , 0.204	Depositor DCC
R_{free} test set	17139 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20344	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, PGE, UJJ, MG, SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/9260	0.44	0/12604
1	B	0.24	0/9251	0.45	0/12595
All	All	0.24	0/18511	0.45	0/25199

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9063	0	9093	46	0
1	B	9042	0	9076	62	0
2	A	58	0	0	0	0
2	B	58	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	2	0
5	A	25	0	0	0	0
5	B	10	0	0	0	0
6	A	10	0	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	30	0	42	4	0
7	B	21	0	30	1	0
8	B	13	0	18	0	0
9	A	983	0	0	8	0
9	B	941	0	0	6	0
All	All	20344	0	18325	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:ND2	9:A:2302:HOH:O	2.15	0.74
1:B:582:THR:HA	6:B:1308:PGE:H2	1.71	0.73
1:A:1183:LEU:O	9:A:2301:HOH:O	2.07	0.72
1:B:452:MET:HE3	1:B:500:VAL:HG21	1.73	0.71
1:B:539:GLU:OE1	9:B:2401:HOH:O	2.09	0.71
1:B:844:CYS:SG	4:B:1303:NAD:C4N	2.82	0.66
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.78	0.66
1:B:788[B]:ARG:HD2	1:B:1187:LEU:HD11	1.78	0.66
1:B:339[B]:VAL:HG21	1:B:350:LEU:HD21	1.77	0.65
1:A:1206:CYS:SG	9:A:3228:HOH:O	2.54	0.65
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.80	0.64
1:A:1095[B]:THR:HG22	9:A:2886:HOH:O	1.98	0.64
1:A:861:LEU:HD22	1:A:865:LYS:HE3	1.80	0.63
1:A:138:ARG:HE	1:A:142[A]:VAL:HG21	1.65	0.62
1:A:557:GLU:OE1	9:A:2303:HOH:O	2.16	0.61
1:B:332:TRP:HZ3	1:B:335:MET:HE2	1.65	0.61
1:B:650:MET:O	1:B:654:LEU:HG	2.01	0.60
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.84	0.59
1:B:358:ARG:HG2	1:B:415:VAL:HG11	1.84	0.59
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.85	0.58
1:A:69:ARG:NH2	1:A:511:ASP:OD1	2.37	0.57
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.34	0.57
1:B:824:LEU:HD23	1:B:827:GLN:HG3	1.87	0.55
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.87	0.55
1:A:844:CYS:SG	4:A:2203:NAD:C4N	2.95	0.55
1:B:937:LEU:HD21	1:B:947:HIS:CD2	2.42	0.55
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.90	0.54
1:A:650:MET:O	1:A:654:LEU:HG	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:TRP:CZ3	1:B:335:MET:HE2	2.43	0.53
1:B:551:LEU:HD22	6:B:1311:PGE:H42	1.90	0.53
1:B:288[B]:ARG:NE	9:B:2409:HOH:O	2.41	0.52
1:B:156:THR:OG1	9:B:2402:HOH:O	2.17	0.51
1:A:367[A]:ARG:NE	1:A:447:GLN:OE1	2.44	0.51
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.46	0.50
1:A:712:ILE:HD13	1:A:781:THR:HG21	1.92	0.50
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.92	0.50
1:A:1226:ASN:O	1:A:1230:MET:HG2	2.11	0.50
1:A:338:VAL:HG22	1:A:367[B]:ARG:HD2	1.94	0.49
1:B:365:MET:HE2	1:B:419:GLN:NE2	2.29	0.48
1:A:202:ARG:NH2	9:A:2321:HOH:O	2.45	0.48
1:B:782:GLY:O	1:B:811:THR:HA	2.13	0.48
1:B:459:GLU:OE1	1:B:465:LYS:NZ	2.44	0.48
1:B:1004:VAL:HG22	7:B:1312:PEG:H42	1.95	0.48
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	1.95	0.47
1:A:202:ARG:NH2	9:A:2324:HOH:O	2.46	0.47
1:A:803:ARG:NH2	1:A:1194:SER:H	2.13	0.47
1:B:338:VAL:HG22	1:B:367:ARG:HB3	1.96	0.47
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.15	0.47
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.50	0.46
1:B:423:HIS:CG	1:B:452:MET:HE2	2.51	0.46
1:B:197:THR:O	1:B:207:ARG:HD2	2.15	0.46
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.51	0.46
1:B:465:LYS:HA	1:B:465:LYS:HD3	1.73	0.46
1:A:223[B]:LEU:HD13	1:A:482:LEU:HA	1.97	0.45
1:A:657:ILE:HD13	1:A:671:GLU:HG2	1.99	0.45
1:A:485:TYR:O	1:A:489:ARG:HG2	2.15	0.45
1:B:370:LYS:NZ	2:B:1301:UJJ:O1A	2.42	0.45
1:B:591[B]:THR:CG2	1:B:601:VAL:HG13	2.47	0.45
1:A:1026:LEU:HD23	1:A:1038:PRO:HG2	1.98	0.45
1:B:844:CYS:SG	4:B:1303:NAD:C3N	3.05	0.45
1:A:132:SER:HB2	1:A:133:HIS:CE1	2.51	0.44
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.99	0.44
1:B:190:MET:HE2	1:B:195:PHE:CZ	2.51	0.44
1:A:485:TYR:CZ	1:A:489:ARG:HD2	2.52	0.44
1:B:338:VAL:HG22	1:B:367:ARG:HD2	1.99	0.44
1:A:1147:LEU:HD22	1:B:1147:LEU:HD22	2.00	0.44
1:A:782:GLY:O	1:A:811:THR:HA	2.18	0.43
1:B:448:CYS:HB2	1:B:453:GLY:HA3	2.00	0.43
1:B:617:VAL:HG12	1:B:774:GLU:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:LEU:HB2	1:A:949:ILE:HG22	2.01	0.43
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.54	0.43
1:B:495:ALA:HB2	1:B:1230:MET:HG3	2.01	0.43
1:B:659:ARG:HD3	9:B:2776:HOH:O	2.18	0.43
1:B:72:ILE:HG22	1:B:510:ILE:HD12	2.01	0.42
1:B:834:THR:O	1:B:838:ASP:HB3	2.18	0.42
1:B:705:PRO:HD3	1:B:781:THR:HB	2.01	0.42
1:B:428:LEU:HD11	1:B:460:VAL:HG21	2.00	0.42
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.55	0.42
1:B:192:GLY:O	1:B:207:ARG:NH1	2.47	0.42
1:B:628:ALA:HB2	1:B:696:PRO:HG3	2.02	0.42
1:B:489:ARG:HA	1:B:489:ARG:NE	2.35	0.42
1:A:375:ASP:OD1	1:A:375:ASP:N	2.48	0.42
1:A:863:MET:HE3	1:A:863:MET:HB2	1.82	0.42
1:A:190:MET:HE2	1:A:190:MET:HB3	1.85	0.41
6:B:1311:PGE:H52	9:B:3190:HOH:O	2.19	0.41
1:B:323:LEU:HB3	1:B:335:MET:HE3	2.01	0.41
1:A:367[B]:ARG:HA	1:A:419:GLN:HB2	2.01	0.41
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.03	0.41
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.45	0.41
1:B:651:PRO:HB3	6:B:1311:PGE:H2	2.03	0.41
1:A:1143:GLN:O	1:A:1147:LEU:HG	2.20	0.41
1:B:290:LYS:NZ	9:B:2410:HOH:O	2.41	0.41
1:B:493:ASN:O	1:B:501:HIS:HB2	2.21	0.41
1:B:918:THR:HB	1:B:923:PHE:CD1	2.56	0.41
1:B:1069:ALA:HA	1:B:1117:ALA:HB1	2.03	0.41
1:B:712:ILE:HD13	1:B:781:THR:HG21	2.02	0.41
1:B:984:HIS:CD2	1:B:984:HIS:C	2.99	0.40
1:A:363:ARG:HA	1:A:415:VAL:O	2.21	0.40
1:B:578:PRO:O	1:B:584:PRO:HA	2.21	0.40
1:B:367:ARG:HA	1:B:419:GLN:HB2	2.03	0.40
1:B:374:TRP:CZ3	1:B:1229:LEU:HG	2.56	0.40
1:A:617:VAL:HG12	1:A:774:GLU:HB2	2.02	0.40
1:A:272:ARG:HB3	1:A:277:GLN:HG3	2.03	0.40
1:A:493:ASN:O	1:A:501:HIS:HB2	2.22	0.40
1:A:878:ARG:HD2	9:A:2643:HOH:O	2.21	0.40
1:B:423:HIS:ND1	1:B:452:MET:HE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1230/1235 (100%)	1204 (98%)	26 (2%)	0	100	100
1	B	1230/1235 (100%)	1204 (98%)	26 (2%)	0	100	100
All	All	2460/2470 (100%)	2408 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	909/951 (96%)	900 (99%)	9 (1%)	68	47
1	B	909/951 (96%)	902 (99%)	7 (1%)	73	56
All	All	1818/1902 (96%)	1802 (99%)	16 (1%)	73	51

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	258	GLU
1	A	321	GLU
1	A	342	TYR
1	A	375	ASP
1	A	730	LYS
1	A	785	GLU
1	A	796	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	934	LEU
1	B	342	TYR
1	B	375[A]	ASP
1	B	375[B]	ASP
1	B	489	ARG
1	B	730	LYS
1	B	934	LEU
1	B	1230	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	685	GLN
1	B	419	GLN
1	B	685	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	2207	-	4,4,4	0.23	0	6,6,6	0.11	0
4	NAD	A	2203	3	46,48,48	3.82	18 (39%)	64,73,73	2.01	12 (18%)
5	SO4	A	2208	-	4,4,4	0.25	0	6,6,6	0.16	0
7	PEG	B	1307	-	6,6,6	0.50	0	5,5,5	0.28	0
5	SO4	A	2205	-	4,4,4	0.25	0	6,6,6	0.09	0
6	PGE	A	2209	-	9,9,9	0.32	0	8,8,8	0.37	0
7	PEG	B	1309	-	6,6,6	0.31	0	5,5,5	0.25	0
2	UJJ	B	1301	-	61,64,64	2.58	22 (36%)	80,98,98	1.97	19 (23%)
5	SO4	B	1305	-	4,4,4	0.22	0	6,6,6	0.07	0
2	UJJ	A	2201	-	61,64,64	2.55	21 (34%)	80,98,98	1.90	15 (18%)
7	PEG	B	1312	-	6,6,6	0.49	0	5,5,5	0.35	0
5	SO4	B	1304	-	4,4,4	0.32	0	6,6,6	0.18	0
8	PG4	B	1310	-	12,12,12	0.51	0	11,11,11	0.18	0
6	PGE	B	1308	-	9,9,9	0.31	0	8,8,8	0.34	0
5	SO4	A	2206	-	4,4,4	0.25	0	6,6,6	0.16	0
6	PGE	B	1311	-	9,9,9	0.32	0	8,8,8	0.32	0
5	SO4	A	2204	-	4,4,4	0.16	0	6,6,6	0.14	0
4	NAD	B	1303	3	46,48,48	3.55	19 (41%)	64,73,73	2.08	14 (21%)
6	PGE	B	1306	-	9,9,9	0.31	0	8,8,8	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	B	1312	-	-	2/4/4/4	-
2	UJJ	B	1301	-	-	4/34/61/61	0/6/7/7
4	NAD	A	2203	3	-	5/30/62/62	0/5/5/5
7	PEG	B	1309	-	-	1/4/4/4	-
6	PGE	B	1308	-	-	1/7/7/7	-
2	UJJ	A	2201	-	-	4/34/61/61	0/6/7/7
7	PEG	B	1307	-	-	0/4/4/4	-
8	PG4	B	1310	-	-	2/10/10/10	-
6	PGE	A	2209	-	-	2/7/7/7	-
6	PGE	B	1311	-	-	5/7/7/7	-
4	NAD	B	1303	3	-	3/30/62/62	0/5/5/5
6	PGE	B	1306	-	-	1/7/7/7	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2203	NAD	O4D-C1D	-10.04	1.27	1.40
2	B	1301	UJJ	PA-O3P	-9.84	1.48	1.59
4	B	1303	NAD	O4D-C1D	-9.83	1.28	1.40
4	A	2203	NAD	PN-O3	9.79	1.70	1.59
2	A	2201	UJJ	PA-O3P	-8.67	1.50	1.59
4	A	2203	NAD	C7N-N7N	8.21	1.48	1.33
4	B	1303	NAD	C3B-C4B	-8.16	1.32	1.53
4	A	2203	NAD	C3B-C4B	-8.16	1.32	1.53
4	B	1303	NAD	C7N-N7N	7.76	1.47	1.33
4	A	2203	NAD	C3D-C4D	-7.57	1.33	1.53
4	B	1303	NAD	PN-O3	7.25	1.67	1.59
4	A	2203	NAD	O4D-C4D	7.12	1.60	1.45
4	B	1303	NAD	C3D-C4D	-6.99	1.35	1.53
4	A	2203	NAD	O4B-C4B	6.97	1.60	1.45
4	B	1303	NAD	O4B-C4B	6.85	1.60	1.45
2	B	1301	UJJ	O4-C4	6.83	1.36	1.23
4	B	1303	NAD	O4D-C4D	6.71	1.59	1.45
2	A	2201	UJJ	O4-C4	6.55	1.36	1.23
4	B	1303	NAD	C6A-N6A	5.91	1.49	1.34
2	B	1301	UJJ	C6-C5X	5.88	1.49	1.39
4	A	2203	NAD	C6A-N6A	5.72	1.48	1.34
2	B	1301	UJJ	O2-C2	5.63	1.35	1.23
2	A	2201	UJJ	C6-C5X	5.53	1.48	1.39
2	A	2201	UJJ	C9-C9A	5.39	1.48	1.39
2	A	2201	UJJ	O2-C2	5.16	1.34	1.23
2	A	2201	UJJ	P-O3P	4.96	1.64	1.59
2	B	1301	UJJ	C9-C9A	4.88	1.47	1.39
4	A	2203	NAD	PA-O3	4.77	1.64	1.59
2	A	2201	UJJ	C4X-N5	4.60	1.45	1.37
4	B	1303	NAD	C3N-C7N	4.31	1.57	1.50
4	A	2203	NAD	O3D-C3D	4.26	1.53	1.43
4	A	2203	NAD	C3N-C7N	4.11	1.56	1.50
2	B	1301	UJJ	C10-N1	4.06	1.44	1.37
2	B	1301	UJJ	C4X-N5	4.06	1.44	1.37
2	A	2201	UJJ	C6A-N6A	3.86	1.44	1.34
4	B	1303	NAD	O3D-C3D	3.85	1.52	1.43
2	B	1301	UJJ	C2-N1	3.81	1.43	1.37
2	B	1301	UJJ	C6A-N6A	3.73	1.43	1.34
4	A	2203	NAD	O4B-C1B	-3.68	1.33	1.42
2	A	2201	UJJ	C2-N1	3.66	1.43	1.37
4	B	1303	NAD	O4B-C1B	-3.63	1.33	1.42
2	A	2201	UJJ	C10-N1	3.63	1.43	1.37
4	B	1303	NAD	C2N-N1N	3.24	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	UJJ	P-O3P	3.20	1.63	1.59
4	B	1303	NAD	O3B-C3B	3.04	1.50	1.43
4	A	2203	NAD	C2N-N1N	2.91	1.38	1.35
2	A	2201	UJJ	C5X-N5	2.91	1.46	1.42
4	A	2203	NAD	O3B-C3B	2.91	1.50	1.43
4	A	2203	NAD	C5A-C4A	-2.66	1.34	1.39
2	A	2201	UJJ	C10-N10	2.65	1.43	1.38
4	A	2203	NAD	C8A-N9A	-2.63	1.33	1.37
4	A	2203	NAD	C2A-N1A	2.61	1.38	1.33
4	B	1303	NAD	C2A-N1A	2.61	1.38	1.33
2	B	1301	UJJ	C10-N10	2.58	1.42	1.38
2	A	2201	UJJ	PA-O5B	-2.58	1.49	1.59
2	B	1301	UJJ	C9A-N10	2.55	1.45	1.41
4	B	1303	NAD	PA-O3	2.41	1.62	1.59
4	A	2203	NAD	O7N-C7N	-2.40	1.19	1.24
2	A	2201	UJJ	C9A-C5X	-2.40	1.36	1.41
2	A	2201	UJJ	O2'-C2'	-2.39	1.38	1.43
2	B	1301	UJJ	C9A-C5X	-2.38	1.36	1.41
2	A	2201	UJJ	C2-N3	2.38	1.41	1.37
2	A	2201	UJJ	C5A-C4A	2.37	1.43	1.39
2	A	2201	UJJ	PA-O2A	-2.35	1.44	1.55
2	B	1301	UJJ	PA-O2A	-2.32	1.44	1.55
2	B	1301	UJJ	C2-N3	2.30	1.41	1.37
2	B	1301	UJJ	PA-O5B	-2.28	1.50	1.59
2	A	2201	UJJ	C4X-C4	2.27	1.49	1.43
2	B	1301	UJJ	C4X-C4	2.26	1.49	1.43
4	B	1303	NAD	O7N-C7N	-2.20	1.20	1.24
2	B	1301	UJJ	C4A-N9A	2.20	1.42	1.37
2	A	2201	UJJ	O3B-C3B	-2.18	1.37	1.43
4	B	1303	NAD	C5A-C4A	-2.17	1.35	1.39
2	A	2201	UJJ	C2B-C3B	-2.17	1.47	1.53
4	B	1303	NAD	C8A-N9A	-2.17	1.33	1.37
2	B	1301	UJJ	P-O1P	2.14	1.58	1.50
4	B	1303	NAD	C8A-N7A	2.12	1.35	1.31
2	B	1301	UJJ	O3B-C3B	-2.12	1.37	1.43
2	B	1301	UJJ	C5A-C4A	2.09	1.42	1.39
2	B	1301	UJJ	O2'-C2'	-2.00	1.39	1.43

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	UJJ	N3A-C2A-N1A	-6.12	119.32	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	UJJ	N3A-C2A-N1A	-6.03	119.46	128.58
4	B	1303	NAD	C5A-C4A-N3A	-5.99	118.47	126.72
4	A	2203	NAD	C4A-N9A-C1B	-5.60	113.53	126.63
2	B	1301	UJJ	O2A-PA-O3P	-5.54	92.30	107.27
4	A	2203	NAD	N3A-C2A-N1A	-5.53	120.21	128.58
4	B	1303	NAD	N9A-C8A-N7A	-5.46	106.19	113.94
4	B	1303	NAD	N3A-C2A-N1A	-5.35	120.48	128.58
4	A	2203	NAD	C5A-C4A-N3A	-5.04	119.78	126.72
4	A	2203	NAD	N9A-C8A-N7A	-5.01	106.83	113.94
2	A	2201	UJJ	C4X-C4-N3	5.00	119.74	110.94
2	A	2201	UJJ	C4-N3-C2	-4.99	119.50	126.37
4	B	1303	NAD	C4A-N9A-C1B	-4.74	115.56	126.63
2	B	1301	UJJ	C5A-C4A-N3A	-4.67	120.28	126.72
4	A	2203	NAD	C4D-O4D-C1D	-4.66	105.66	109.92
4	B	1303	NAD	N3A-C4A-N9A	4.64	135.06	127.17
2	A	2201	UJJ	C5A-C4A-N3A	-4.45	120.59	126.72
2	B	1301	UJJ	C4-N3-C2	-4.42	120.28	126.37
2	B	1301	UJJ	N3-C2-N1	4.33	122.55	115.74
2	B	1301	UJJ	N3A-C4A-N9A	4.31	134.50	127.17
4	A	2203	NAD	C1B-N9A-C8A	4.26	136.56	127.09
4	B	1303	NAD	C4D-O4D-C1D	-4.21	106.07	109.92
4	B	1303	NAD	C4A-N9A-C8A	4.21	110.16	105.74
2	B	1301	UJJ	C4X-C4-N3	4.18	118.29	110.94
4	A	2203	NAD	N3A-C4A-N9A	4.02	134.01	127.17
2	A	2201	UJJ	C5A-N7A-C8A	4.02	109.77	103.45
4	A	2203	NAD	C4A-N9A-C8A	3.95	109.89	105.74
2	A	2201	UJJ	N3A-C4A-N9A	3.81	133.64	127.17
2	A	2201	UJJ	N3-C2-N1	3.78	121.68	115.74
4	B	1303	NAD	C5A-N7A-C8A	3.78	109.38	103.45
4	B	1303	NAD	C2A-N3A-C4A	3.75	120.99	111.83
2	B	1301	UJJ	C5A-N7A-C8A	3.59	109.10	103.45
2	B	1301	UJJ	O3P-PA-O1A	3.54	121.36	110.70
2	B	1301	UJJ	C2A-N3A-C4A	3.50	120.37	111.83
2	A	2201	UJJ	N9A-C8A-N7A	-3.47	109.01	113.94
2	A	2201	UJJ	O2A-PA-O3P	-3.46	97.93	107.27
2	A	2201	UJJ	C2A-N3A-C4A	3.45	120.27	111.83
2	B	1301	UJJ	C5X-N5-C4X	-3.42	111.98	120.01
2	A	2201	UJJ	C5X-N5-C4X	-3.33	112.20	120.01
4	A	2203	NAD	C5A-N7A-C8A	3.28	108.60	103.45
2	A	2201	UJJ	C4A-C5A-N7A	-3.25	106.86	110.58
4	B	1303	NAD	C1B-N9A-C8A	3.24	134.28	127.09
4	A	2203	NAD	C2A-N3A-C4A	3.23	119.71	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	UJJ	N9A-C8A-N7A	-3.13	109.50	113.94
2	B	1301	UJJ	C2A-N1A-C6A	2.78	123.30	118.73
2	B	1301	UJJ	C6-C5X-N5	-2.72	117.50	121.89
2	A	2201	UJJ	C4A-N9A-C8A	2.71	108.59	105.74
2	A	2201	UJJ	C2A-N1A-C6A	2.71	123.18	118.73
2	A	2201	UJJ	O4-C4-C4X	-2.56	121.33	127.62
4	A	2203	NAD	C2N-C3N-C4N	2.52	121.19	118.26
2	B	1301	UJJ	O2-C2-N1	-2.46	117.50	121.86
4	B	1303	NAD	C4A-C5A-N7A	-2.42	107.82	110.58
4	B	1303	NAD	C6A-C5A-C4A	2.35	120.38	117.18
2	B	1301	UJJ	O4-C4-C4X	-2.34	121.87	127.62
4	A	2203	NAD	C6A-C5A-C4A	2.31	120.33	117.18
2	B	1301	UJJ	C4A-N9A-C8A	2.31	108.16	105.74
4	B	1303	NAD	C2B-C1B-N9A	-2.29	107.62	113.30
2	B	1301	UJJ	C4A-C5A-N7A	-2.23	108.03	110.58
4	B	1303	NAD	C3N-C7N-N7N	2.08	120.30	117.74
2	B	1301	UJJ	C4A-N9A-C1B	-2.07	121.80	126.63

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2203	NAD	C5B-O5B-PA-O1A
6	A	2209	PGE	O1-C1-C2-O2
6	B	1311	PGE	O1-C1-C2-O2
7	B	1312	PEG	O2-C3-C4-O4
6	B	1306	PGE	O1-C1-C2-O2
2	A	2201	UJJ	C2'-C3'-C4'-O4'
8	B	1310	PG4	C8-C7-O4-C6
6	B	1311	PGE	C1-C2-O2-C3
6	B	1311	PGE	C4-C3-O2-C2
4	A	2203	NAD	C2B-C1B-N9A-C8A
4	B	1303	NAD	C2B-C1B-N9A-C8A
4	B	1303	NAD	C4D-C5D-O5D-PN
4	B	1303	NAD	C5B-O5B-PA-O1A
4	A	2203	NAD	C4D-C5D-O5D-PN
7	B	1309	PEG	C1-C2-O2-C3
8	B	1310	PG4	C6-C5-O3-C4
6	B	1311	PGE	O3-C5-C6-O4
7	B	1312	PEG	C4-C3-O2-C2
6	B	1311	PGE	C3-C4-O3-C5
2	A	2201	UJJ	PA-O3P-P-O1P

Continued on next page...

Continued from previous page...

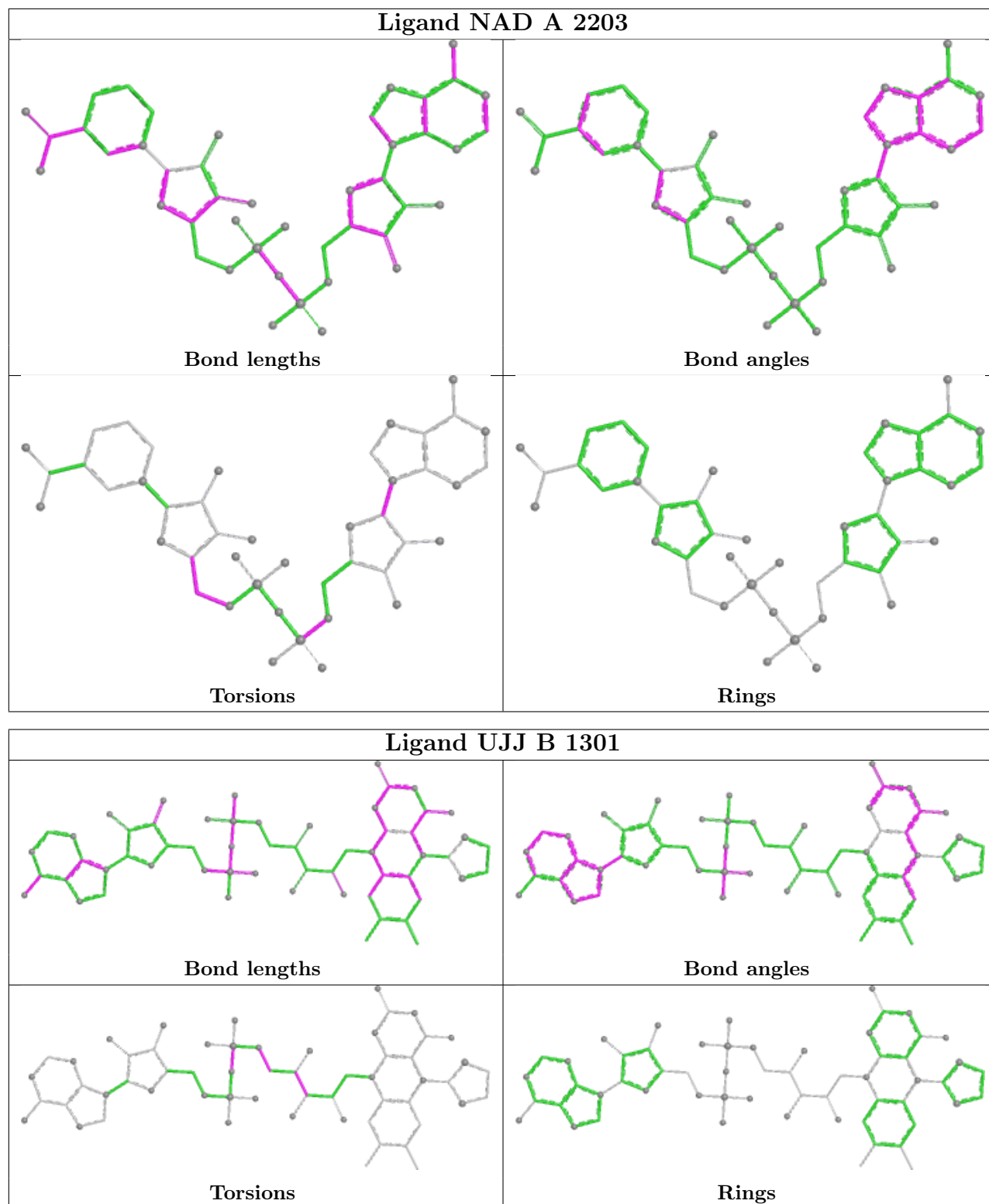
Mol	Chain	Res	Type	Atoms
2	B	1301	UJJ	PA-O3P-P-O1P
4	A	2203	NAD	C3D-C4D-C5D-O5D
2	A	2201	UJJ	C4'-C5'-O5'-P
6	A	2209	PGE	C4-C3-O2-C2
2	A	2201	UJJ	PA-O3P-P-O2P
2	B	1301	UJJ	PA-O3P-P-O2P
2	B	1301	UJJ	C2'-C3'-C4'-O4'
4	A	2203	NAD	C2B-C1B-N9A-C4A
6	B	1308	PGE	O3-C5-C6-O4
2	B	1301	UJJ	C4'-C5'-O5'-P

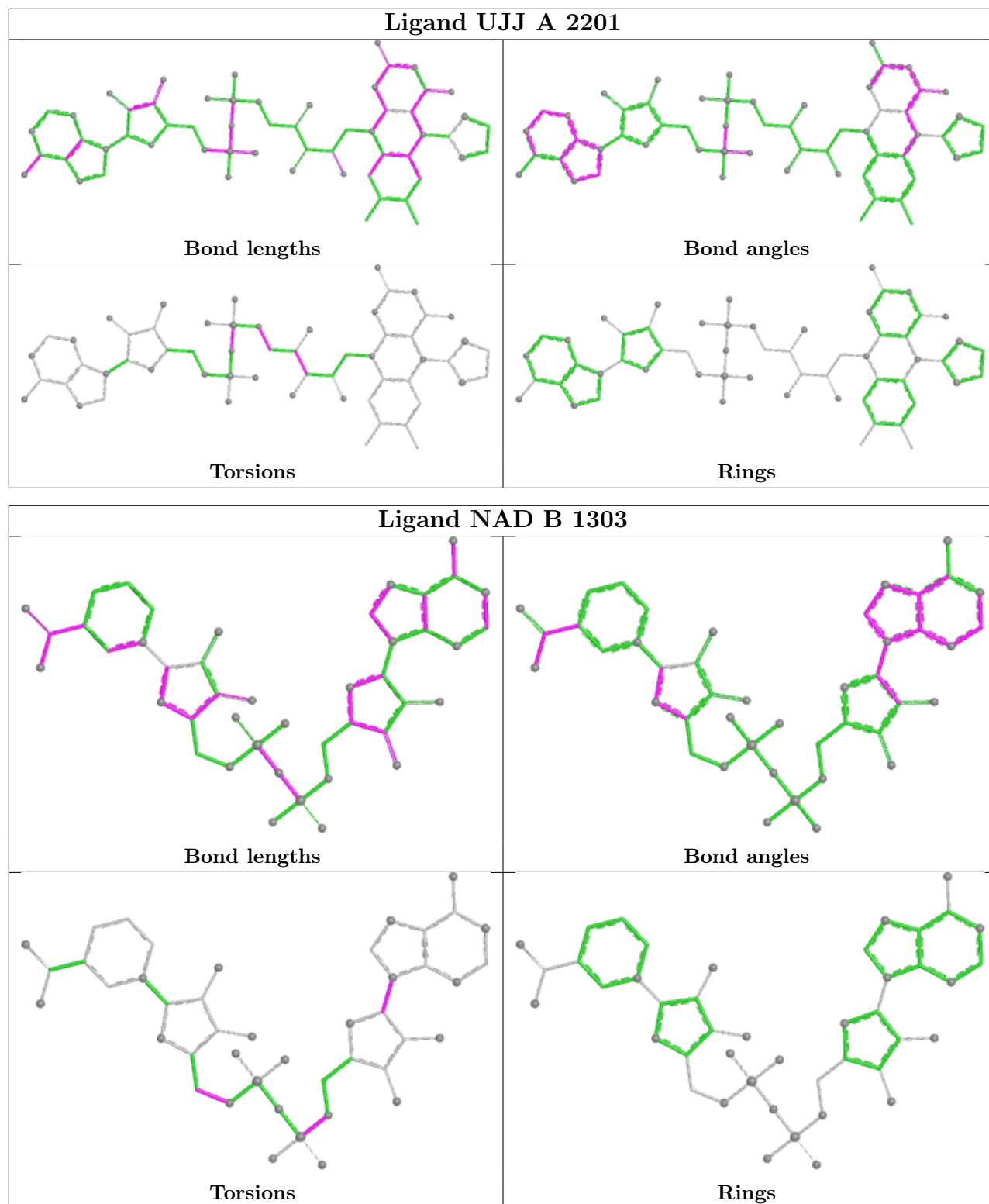
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2203	NAD	1	0
2	B	1301	UJJ	1	0
7	B	1312	PEG	1	0
6	B	1308	PGE	1	0
6	B	1311	PGE	3	0
4	B	1303	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1217/1235 (98%)	0.14	64 (5%)	32	39	8, 21, 48, 86	17 (1%)
1	B	1217/1235 (98%)	0.22	94 (7%)	19	23	8, 22, 48, 83	15 (1%)
All	All	2434/2470 (98%)	0.18	158 (6%)	25	29	8, 21, 48, 86	32 (1%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1222	ALA	6.5
1	A	195	PHE	6.2
1	B	912	ILE	5.9
1	A	482	LEU	5.8
1	B	195	PHE	5.6
1	A	1002	GLY	5.5
1	A	483	LEU	5.0
1	B	1233	GLY	5.0
1	B	1223	ALA	5.0
1	B	490	LEU	4.8
1	B	483	LEU	4.8
1	B	486	LEU	4.7
1	B	482	LEU	4.6
1	B	14	ALA	4.3
1	B	133	HIS	4.3
1	B	80	SER	4.2
1	A	191	MET	4.0
1	A	490	LEU	4.0
1	B	192	GLY	3.9
1	A	224[A]	GLY	3.9
1	A	129	ASN	3.9
1	B	485	TYR	3.9
1	B	481	THR	3.9
1	A	192	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	481	THR	3.8
1	B	439	PHE	3.8
1	B	138	ARG	3.8
1	B	84	VAL	3.7
1	A	80	SER	3.7
1	B	134	LEU	3.7
1	A	497	SER	3.7
1	A	479	HIS	3.7
1	B	491	LEU	3.6
1	B	1232	ILE	3.6
1	B	224	GLY	3.6
1	B	79	HIS	3.5
1	A	1231	ALA	3.5
1	A	119	ALA	3.5
1	B	478	THR	3.5
1	A	496	ASN	3.4
1	B	913	GLY	3.4
1	B	918	THR	3.3
1	A	1232	ILE	3.3
1	B	496	ASN	3.3
1	B	506	PRO	3.2
1	B	1230	MET	3.2
1	B	223	LEU	3.2
1	B	495	ALA	3.2
1	A	506	PRO	3.1
1	A	79	HIS	3.1
1	A	134	LEU	3.1
1	B	497	SER	3.0
1	A	130	TRP	3.0
1	A	491	LEU	3.0
1	A	116	THR	3.0
1	A	486	LEU	3.0
1	B	914	LEU	3.0
1	B	129	ASN	3.0
1	A	478	THR	3.0
1	B	156	THR	3.0
1	A	796	ASP	3.0
1	A	138	ARG	3.0
1	A	1233	GLY	2.9
1	A	223[A]	LEU	2.9
1	A	1222	ALA	2.9
1	A	125	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	194	GLN	2.9
1	A	115	ALA	2.8
1	A	801	ALA	2.8
1	B	1227	ALA	2.8
1	B	479	HIS	2.8
1	A	503	ILE	2.8
1	A	14	ALA	2.8
1	A	1223	ALA	2.8
1	B	480	GLU	2.8
1	B	484	ALA	2.8
1	B	462	GLY	2.8
1	B	508	VAL	2.7
1	A	113	ASP	2.7
1	A	133	HIS	2.7
1	B	501	HIS	2.7
1	A	1003	ALA	2.7
1	B	194	GLN	2.7
1	B	1231	ALA	2.6
1	B	191	MET	2.6
1	B	124	LYS	2.6
1	A	81	GLY	2.6
1	B	915	ALA	2.6
1	B	75	LEU	2.6
1	B	494	GLY	2.6
1	A	485	TYR	2.5
1	B	905	LEU	2.5
1	B	81	GLY	2.5
1	B	493	ASN	2.5
1	B	510	ILE	2.5
1	B	1224	GLY	2.5
1	B	74	ALA	2.5
1	B	503	ILE	2.5
1	A	77	GLY	2.5
1	B	132	SER	2.5
1	A	84	VAL	2.5
1	A	451	GLY	2.4
1	B	438	ASP	2.4
1	A	114	THR	2.4
1	B	83	GLY	2.4
1	B	1229	LEU	2.4
1	A	82	SER	2.4
1	B	800	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	236	TYR	2.4
1	A	190	MET	2.4
1	B	452	MET	2.4
1	B	221	ASP	2.3
1	B	463	ARG	2.3
1	B	131	LYS	2.3
1	A	1228	SER	2.3
1	B	330	SER	2.3
1	B	116	THR	2.3
1	A	131	LYS	2.3
1	A	937	LEU	2.3
1	A	120	LEU	2.3
1	B	82	SER	2.3
1	A	484	ALA	2.2
1	B	64	ALA	2.2
1	B	1226	ASN	2.2
1	A	508	VAL	2.2
1	B	130	TRP	2.2
1	B	63	ALA	2.2
1	B	505	ASP	2.2
1	A	128	GLY	2.2
1	B	451	GLY	2.2
1	B	487	VAL	2.2
1	B	1059	GLY	2.2
1	B	1225	GLY	2.2
1	A	912	ILE	2.1
1	B	916	SER	2.1
1	A	127	ASP	2.1
1	B	196	VAL	2.1
1	B	520	VAL	2.1
1	B	489	ARG	2.1
1	B	155	LEU	2.1
1	B	111	ILE	2.1
1	B	500	VAL	2.1
1	A	1230	MET	2.1
1	B	410	LEU	2.1
1	A	189	ARG	2.1
1	B	189	ARG	2.1
1	B	66	SER	2.1
1	B	112	PRO	2.1
1	B	415	VAL	2.0
1	B	440	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	188	MET	2.0
1	A	1224	GLY	2.0
1	A	112	PRO	2.0
1	B	200	THR	2.0
1	B	523	ALA	2.0
1	A	500	VAL	2.0
1	B	499	PHE	2.0
1	B	1228	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	1305	5/5	0.67	0.17	100,102,102,104	0
5	SO4	A	2205	5/5	0.80	0.16	61,61,64,72	0
6	PGE	B	1311	10/10	0.81	0.19	47,56,63,67	0
5	SO4	A	2206	5/5	0.83	0.12	54,56,61,64	0
6	PGE	B	1308	10/10	0.84	0.14	33,47,62,66	0
5	SO4	A	2208	5/5	0.86	0.14	64,69,75,80	0
7	PEG	B	1312	7/7	0.87	0.15	23,44,50,51	0
5	SO4	A	2207	5/5	0.88	0.10	71,72,74,78	0
6	PGE	A	2209	10/10	0.89	0.12	23,38,47,51	0
8	PG4	B	1310	13/13	0.89	0.14	40,51,57,58	0
7	PEG	B	1307	7/7	0.90	0.14	40,42,51,53	0
7	PEG	B	1309	7/7	0.90	0.11	27,28,35,42	0
6	PGE	B	1306	10/10	0.91	0.11	27,40,45,48	0
3	MG	B	1302	1/1	0.95	0.11	27,27,27,27	0
4	NAD	A	2203	44/44	0.95	0.07	18,22,28,30	0

Continued on next page...

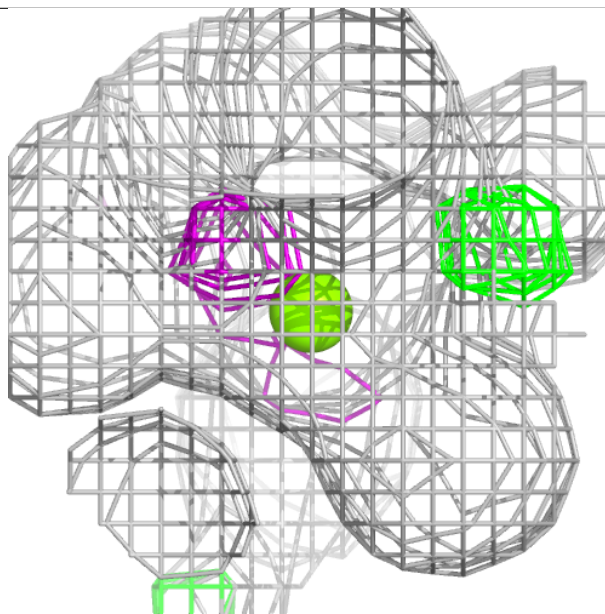
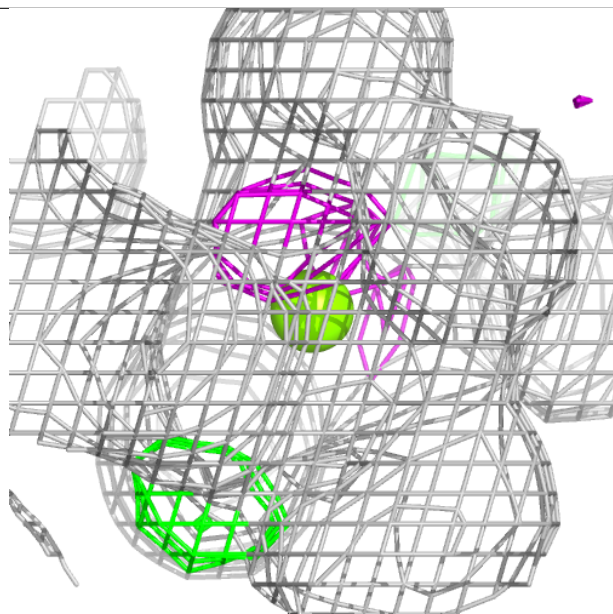
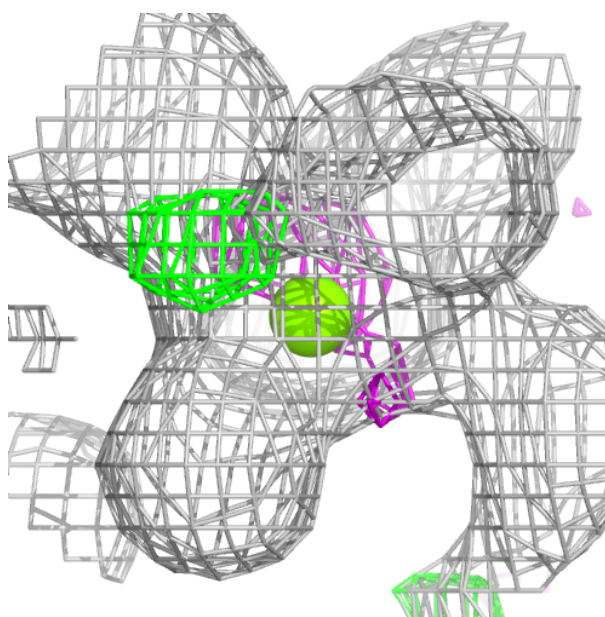
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	2202	1/1	0.95	0.08	32,32,32,32	0
2	UJJ	B	1301	58/58	0.96	0.07	16,21,26,31	0
4	NAD	B	1303	44/44	0.97	0.06	13,16,20,32	0
2	UJJ	A	2201	58/58	0.97	0.05	13,19,24,32	0
5	SO4	B	1304	5/5	0.99	0.04	15,19,23,24	0
5	SO4	A	2204	5/5	0.99	0.04	17,19,22,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

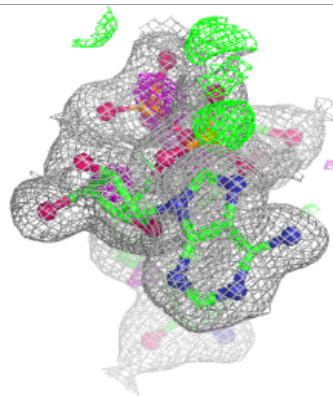
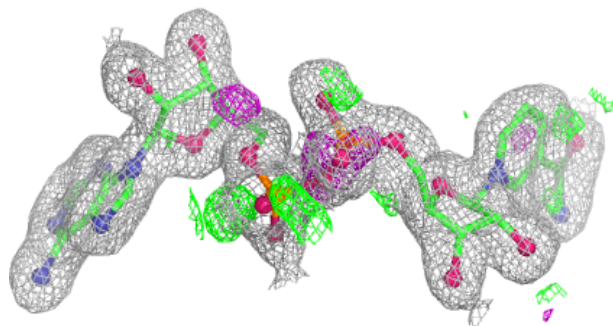
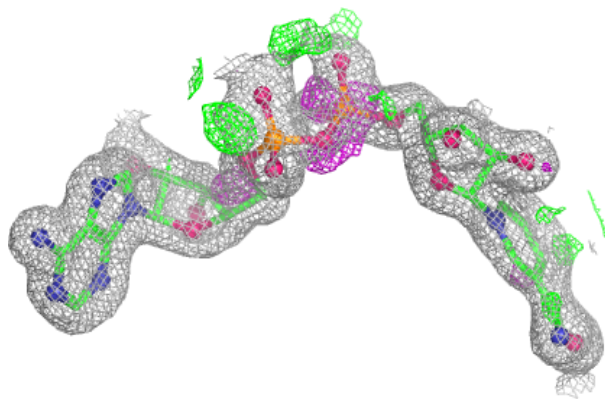
Electron density around MG B 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



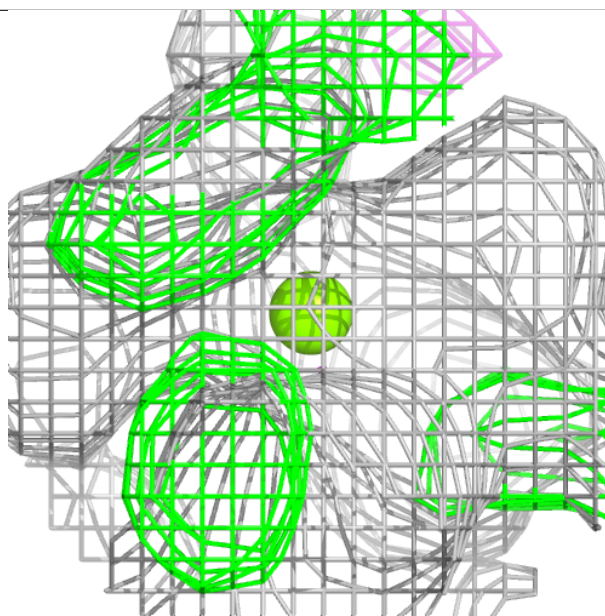
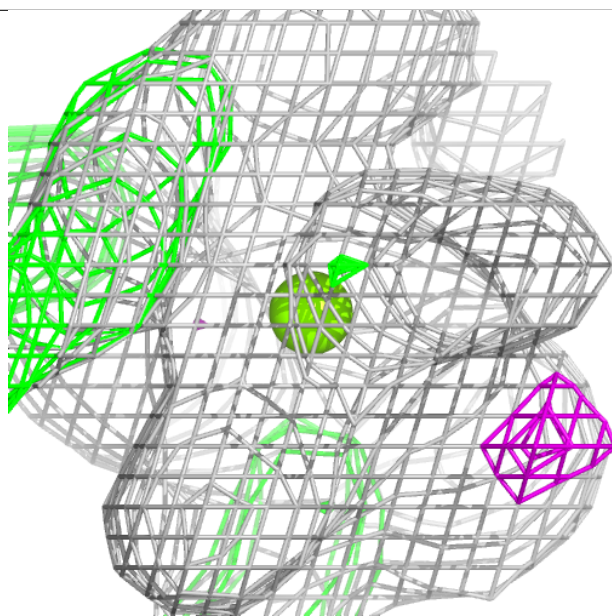
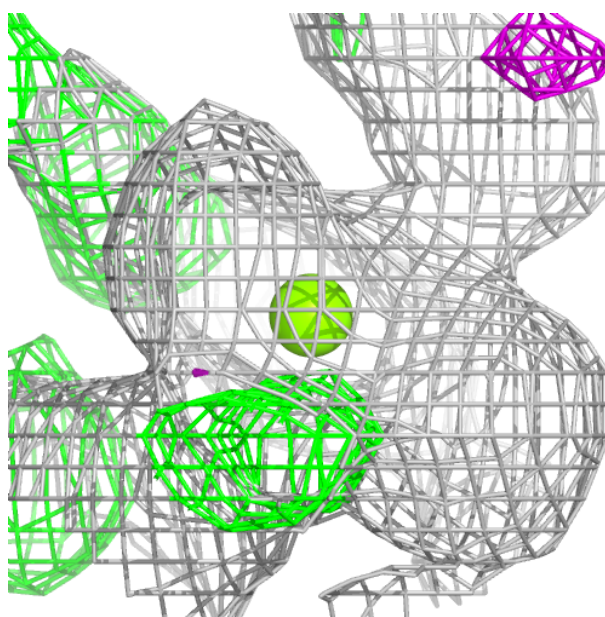
Electron density around NAD A 2203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



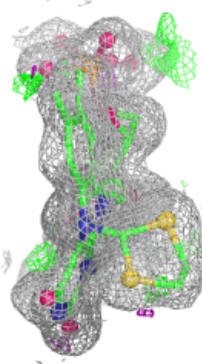
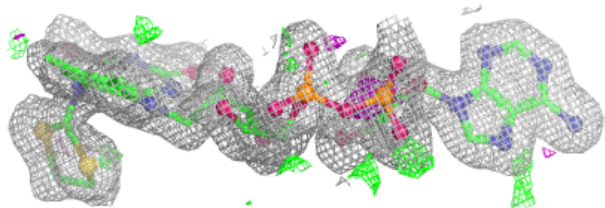
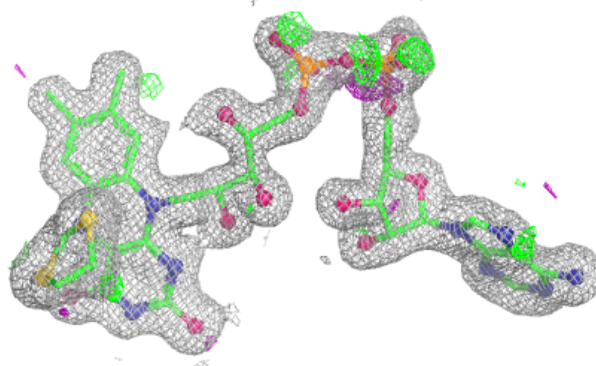
Electron density around MG A 2202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

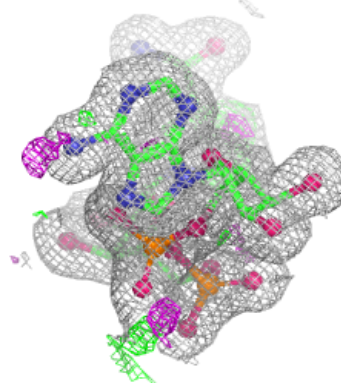
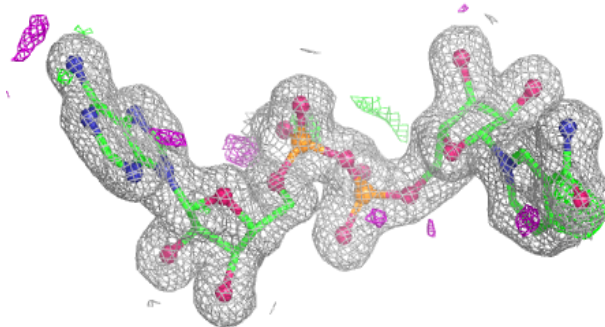
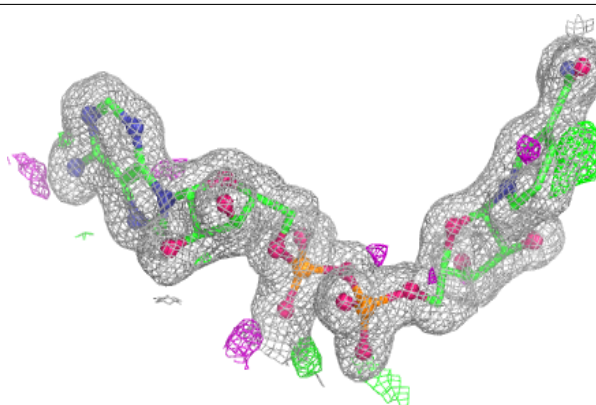


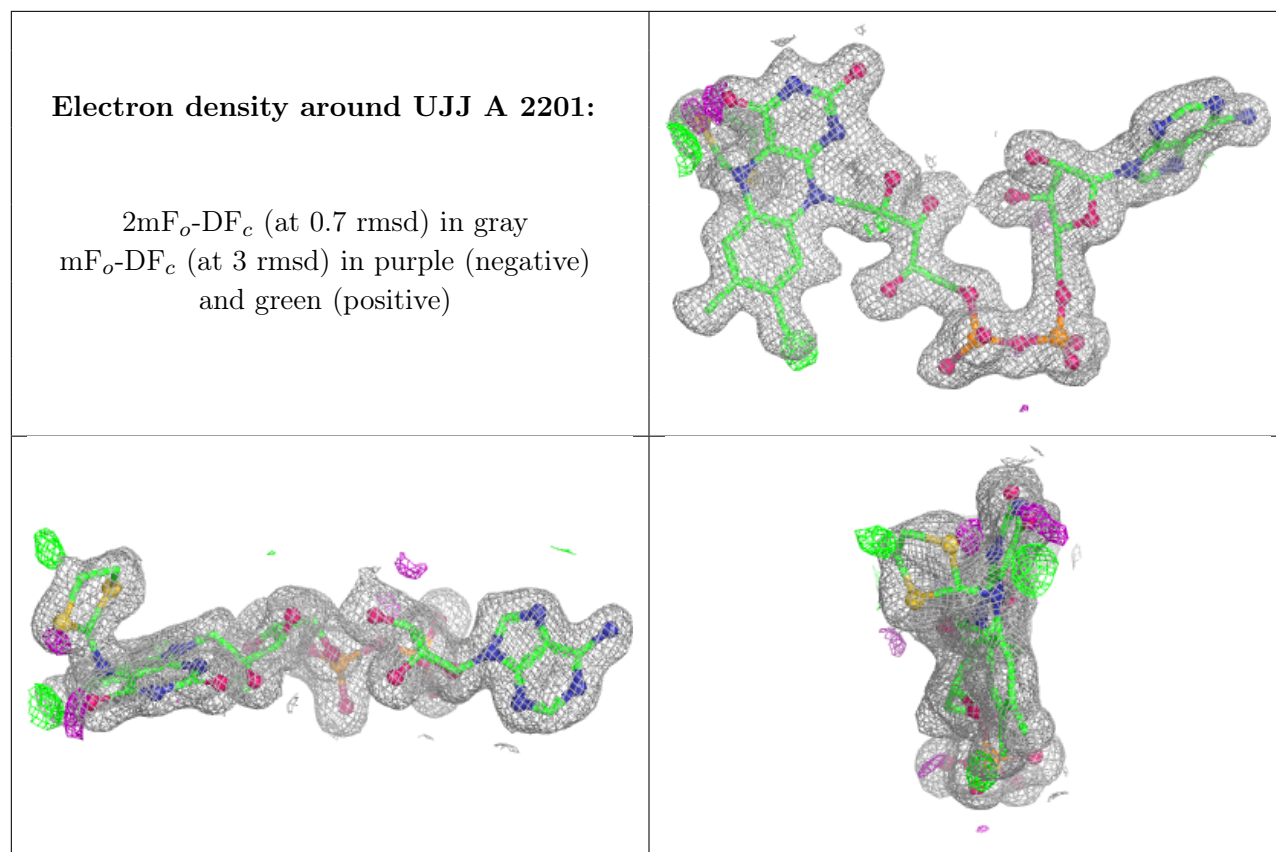
Electron density around UJJ B 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD B 1303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.